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PCT Int. Appl., 92 pp.
SO
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                                                                     19961220
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                                 19970710
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             MR, NE, SN, TD, TG
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                                 19961227
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     US 1996-782894
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     US 1999-270734
                           A3
                                 20000211
     US 2000-502005
     MARPAT 127:135646
os
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Ι

inhibitors, especially for thrombin, factor Xa, trypsin, and chymotrypsin. Thus, isonipecotic acid was converted to its N-tert-butoxycarbonyl derivative and reduced to N-tert-butoxycarbonyl-4-piperidinemethanol, which was treated with 2-ClC6H4SO3C6H3(OH)Me-3,5,followed by deblocking, reaction with MeC(NH)OEt.HCl to give the imidate I. I had a Ki for thrombin inhibition of 1.65  $\mu M$ .

IT193096-44-5P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of amidine derivs. as selective protease inhibitors)

193096-44-5 CAPLUS RN

Benzenesulfonic acid, 2-chloro-, 3-[[4-(aminoiminomethyl)phenyl]methoxy]-5-CNmethylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N-C} \\ & \\ \text{CH}_2\text{-O} \\ & \\ \text{Me} \\ \end{array}$$

#### HCl

```
L13 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2004 ACS on STN
     1997:342428 CAPLUS
AN
DN
     126:317391
     Preparation of [(N-amidinoazinyl)alkoxy]phenyl benzenesulfonates and
TI
     analogs as protease inhibitors
     Lu, Tianbao; Illig, Carl R.; Tomczuk, Bruce E.; Soll, Richard M.;
     Subasinghe, Nalin L.; Bone, Roger F.
     3-Dimensional Pharmaceuticals, Inc., USA
PΑ
     PCT Int. Appl., 144 pp.
SO
     CODEN: PIXXD2
DТ
     Patent
     English
LΑ
FAN.CNT 2
                                                                    DATE
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19960927
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    NO 9801393
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PRAI US 1995-536939
                          Α
                                19960815
                          Α
    US 1996-698401
                                19960927
                          W
     WO 1996-US15609
    MARPAT 126:317391
OS
     R1ZZ1Z2(CH2)nZ3(CH2)mNR8C(:NRa)NRbRc[I; R1 = alk(en)yl, aryl(alkyl),
AB
     heteroaryl, etc.; Z = NR10SO2, SO2O, NR10CO, etc.; Z1 = (un) substituted
     phenylene; Z2 = bond, O, S, (alkyl)imino, alkylidene, etc.; Z3 = NR7 or
     CR7R10; R7,R8 = H, alkyl, aryl(alkyl), etc.; R7R8 = bond, CH2, CH2CH2; R10
     = H, (alkoxy)alkyl, aryl(alkyl), etc.; Ra-Rc = H, OH, cyano, alkyl,
     alkoxy(carbonyl), etc.; m = 1-5; n = 0-8] were prepared Thus, 3-(HO)C6H4OAc
     was converted in 2 steps to 3-(HO)C6H4OCH2Ph which was esterified by
     2-ClC6H4SO2Cl and the deprotected product etherified by
     N-tert-butoxycarbonyl-4-piperidinylmethyl methanesulfonate to give, in 2
     addnl. steps, 2-ClC6H4SO2OC6H4(OCH2R)-3 (R = 1-amidino-4-piperidinyl).
     Data for biol. activity of I were given.
     189338-84-9P 189338-86-1P 189338-92-9P
IT
     189338-99-6P 189339-01-3P 189339-07-9P
     189339-09-1P 189339-11-5P 189339-13-7P
     189339-14-8P 189339-15-9P 189339-16-0P
     189339-17-1P 189339-18-2P 189339-19-3P
     189339-20-6P 189339-21-7P 189339-22-8P
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     189339-29-5P 189339-31-9P 189339-32-0P
     189339-33-1P 189339-35-3P 189339-37-5P
     189339-38-6P 189339-40-0P 189339-41-1P
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     189339-45-5P 189339-46-6P 189339-47-7P
     189339-48-8P 189339-49-9P 189339-50-2P
     189339-51-3P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of [(N-amidinoazinyl)alkoxy]phenyl benzenesulfonates and
        analogs as protease inhibitors)
     189338-84-9 CAPLUS
RN
     Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-
CN
     piperidinyl]methoxy]phenyl ester (9CI) (CA INDEX NAME)
```

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N}-\text{C} \\ & \\ & \\ \text{CH}_2-\text{O} \\ & \\ & \\ & \\ \end{array}$$

RN 189338-86-1 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ \text{N} \\ \text{CH}_2-\text{O} \\ \text{Me} \\ \end{array}$$

RN 189338-92-9 CAPLUS
CN Benzoic acid, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-[[(2-chlorophenyl)sulfonyl]oxy]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N-C} \\ & \\ \text{N} \\ & \\ \text{CH}_2\text{-O} \\ & \\ \text{O} \\ & \\ \text{O} \\ \end{array}$$

RN 189338-99-6 CAPLUS
CN 1-Piperidinecarboximidamide, 4-[[[3-[(phenylmethyl) (phenylsulfonyl)amino]p
henyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \text{||} \\ \text{C-NH}_2 \\ & \text{N-CH}_2 - \text{Ph} \\ \text{O-S-Ph} \\ & \text{||} \\ & \text{O} \end{array}$$

RN 189339-01-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-4-(phenylmethyl)phenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-00-2 CMF C26 H28 Cl N3 O4 S

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N-C} \\ & \\ \text{N} \\ & \\ \text{CH}_2\text{-O} \\ & \\ \text{O} \\ & \\ \text{O}$$

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN 189339-07-9 CAPLUS
CN 1-Naphthalenesulfonic acid, 3-[[1-(aminoiminomethyl)-4piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-06-8 CMF C24 H27 N3 O4 S

$$\begin{array}{c|c} & & & \\ & & & \\ H_2N-C & & & \\ & & & \\ NH & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN 189339-09-1 CAPLUS

Benzenesulfonic acid, 3-(trifluoromethyl)-, 3-[[1-(aminoiminomethyl)-4piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-08-0 CMF C21 H24 F3 N3 O4 S

$$\begin{array}{c|c} & \text{NH} \\ \parallel \\ \parallel \\ \text{CH}_2\text{N} - \text{C} \\ & \text{CH}_2 - \text{O} \\ & \text{Me} \\ \end{array}$$

CM2

64-19-7 CRN CMF C2 H4 O2

189339-11-5 CAPLUS RN

1-Piperidinecarboximidamide, 4-[[3-methyl-5-[(phenylsulfonyl)oxy]phenoxy]m CNethyl]-, monoacetate (9CI) (CA INDEX NAME)

CM 1

189339-10-4 CRN CMF C20 H25 N3 O4 S

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{C-NH}_2 \\ \text{O} \\ \text{Ph-S-O} \\ \text{O} \end{array}$$

CM2

CRN 64-19-7

CMF C2 H4 O2

RN 189339-13-7 CAPLUS

Benzenesulfonic acid, 3-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-12-6 CMF C20 H24 Cl N3 O4 S

$$\begin{array}{c|c} NH \\ \parallel \\ H_2N-C \\ \hline \\ N \\ CH_2-O \\ \hline \\ CH_2-O \\ \hline \\ \\ O \\ C1 \\ \end{array}$$

CM 2

CRN 64-19-7 CMF C2 H4 O2

RN 189339-14-8 CAPLUS
CN Benzenesulfonic acid, 3-methoxy-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN

189339-15-9 CAPLUS Acetic acid, [3-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-CN methylphenoxy]sulfonyl]phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \text{H}_2\text{N-C} \\ \text{N} \\ \text{CH}_2\text{-O} \\ \text{O} \\ \text{Me} \\ \end{array}$$

189339-16-0 CAPLUS RN

Benzenesulfonic acid, 3-hydroxy-, 3-[[1-(aminoiminomethyl)-4piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N-C} \\ \text{N} \\ \text{CH}_2\text{-O} \\ \text{O} \\ \text{Me} \\ \end{array}$$

● HCl

189339-17-1 CAPLUS RN

Benzenesulfonic acid, 3-(2-hydroxyethoxy)-, 3-[[1-(aminoiminomethyl)-4-CNpiperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N}-\text{C} \\ & \\ \text{N} \\ & \\ \text{CH}_2-\text{O} \\ & \\ \text{O} \\ & \\ \text{CH}_2-\text{CH}_2-\text{OH}_2 \\ \\ & \\ \text{O} \\ & \\ \text{O$$

● HCl

RN 189339-18-2 CAPLUS
CN Benzenesulfonic acid, 3-(2,3-dihydroxypropoxy)-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 189339-19-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-chlorophenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N-C} \\ & \\ & \\ \text{CH}_2\text{-O} \\ & \\ & \\ & \\ \text{C1} \\ \end{array}$$

• HCl

RN 189339-20-6 CAPLUS
CN Benzenesulfonic acid, 3-nitro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ \text{N} \\ \text{CH}_2-\text{O} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{O} \\ \text{N} \\ \text{O} \\ \text{O} \\ \text{N} \\ \text{O} \\$$

HCl

RN 189339-21-7 CAPLUS
CN Benzenesulfonic acid, 3-amino-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ \text{N} \\ \text{CH}_2-\text{O} \\ \text{Me} \\ \end{array}$$

● HCl

RN 189339-22-8 CAPLUS
CN Benzoic acid, 3-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5methylphenoxy]sulfonyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX
NAME)

● HCl

RN 189339-23-9 CAPLUS CN Benzenesulfonic acid, 4-nitro-, 3-[[1-(aminoiminomethyl)-4-

piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & NH \\ \parallel \\ H_2N-C \\ \hline \\ NO_2 \\ \hline \\ CH_2-O \\ \hline \\ O \\ \\ Me \\ \end{array}$$

● HCl

RN 189339-24-0 CAPLUS
CN Benzenesulfonic acid, 4-amino-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CFINDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ & \text{N} \\ & \text{CH}_2-\text{O} \\ & \text{Me} \\ \end{array}$$

● HCl

RN 189339-25-1 CAPLUS
CN Benzenesulfonic acid, 2-nitro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \text{H}_2\text{N-C} \\ \text{N} \\ \text{CH}_2\text{-O} \\ \text{Me} \end{array}$$

189339-26-2 CAPLUS RN

Benzenesulfonic acid, 2-amino-, 3-[[1-(aminoiminomethyl)-4-CN piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NH \\ H_2N-C \\ N \\ CH_2-O \\ O \\ Me \\ \end{array}$$

## ● HCl

189339-27-3 CAPLUS RN

Benzenesulfonic acid, 2-chloro-3-nitro-, 3-[[1-(aminoiminomethyl)-4-CNpiperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

189339-28-4 CAPLUS

Benzenesulfonic acid, 3-amino-2-chloro-, 3-[[1-(aminoiminomethyl)-4piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} NH \\ \parallel \\ H_2N-C \\ N \\ CH_2-O \\ \hline \\ O \\ C1 \\ NH_2 \\ \end{array}$$

● HCl

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N-C} \\ & \\ \text{N} \\ & \\ \text{CH}_2\text{-O} \\ & \\ \text{O} \\ & \\ \text{Me} \\ & \\ \text{C} \\ & \\ \text{O} \\ & \\ \text{C} \\ & \\ \text{O} \\ \\ \end{array}$$

● HCl

RN 189339-31-9 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 4-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-2-naphthalenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-30-8 CMF C23 H24 Cl N3 O4 S

CM2

CRN 64-19-7 C2 H4 O2 CMF

189339-32-0 CAPLUS RN

Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methoxyphenyl ester (9CI) (CA INDEX NAME) CN

189339-33-1 CAPLUS RN

Benzoic acid, 2-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-4-[[(2-chlorophenyl)sulfonyl]oxy]-6-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \text{H}_2\text{N-C} \\ \text{N} \\ \text{EtO-C} \\ \text{O} \\ \text{Me} \\ \end{array}$$

### HCl

189339-35-3 CAPLUS RN

Benzenesulfonic acid, 2-(trifluoromethyl)-, 3-[[1-(aminoiminomethyl)-4-CNpiperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 189339-34-2 CMF C21 H24 F3 N3 O4 S

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N-C} \\ & \\ \text{N} \\ & \\ \text{CH}_2\text{--}0 \\ & \\ & \\ \text{Me} \\ \end{array}$$

CM

64-19-7 CRN CMF C2 H4 O2

189339-37-5 CAPLUS RN

Benzenesulfonic acid, 3-methyl-, 3-[[1-(aminoiminomethyl)-4-CN piperidinyl]methoxy]-5-methylphenyl ester, monoacetate (9CI) NAME)

CM 1

CRN 189339-36-4 CMF C21 H27 N3 O4 S

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N-C} \\ \text{N} \\ \text{CH}_2\text{-O} \\ \text{O} \\ \text{Me} \\ \end{array}$$

2 CM

CRN 64-19-7 CMF C2 H4 O2

189339-38-6 CAPLUS RNBenzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-ethylphenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ \\ \text{CH}_2-\text{O} \\ \\ \text{Et} \\ \end{array}$$

## ● HCl

189339-40-0 CAPLUS

Benzenesulfonic acid, 2,3-dichloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl ester, monohydrochloride (9CI) (CA CNINDEX NAME)

$$\begin{array}{c|c} NH \\ \parallel \\ H_2N-C \\ \hline \\ CH_2-O \\ \hline \\ \\ Me \\ \end{array}$$

● HCl

RN 189339-41-1 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-1-naphthalenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

● HCl

RN 189339-42-2 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-(hydroxymethyl)phenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH} \\ & \\ \text{H}_2\text{N}-\text{C} \\ & \\ \text{N} \\ & \\ \text{CH}_2-\text{O} \\ & \\ & \\ \text{HO}-\text{CH}_2 \\ \end{array}$$

189339-43-3 CAPLUS RN

Glycine, N-[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-(trifluoromethyl)phenyl]-N-[(2-chlorophenyl)sulfonyl]-, monohydrochloride CN (9CI) (CA INDEX NAME)

## ● HCl

189339-44-4 CAPLUS RN

Hexanoic acid, 6-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl][(2-chlorophenyl)sulfonyl]amino]-, methyl ester, CN monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} NH & & & & & \\ NH & & & & & \\ H_2N-C & & & & \\ N & & & & \\ CH_2-O & & & & \\ N-S & & & \\ Me & & & \\ \end{array}$$

## HC1

189339-45-5 CAPLUS RN

Hexanoic acid, 6-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-methylphenyl][(2-chlorophenyl)sulfonyl]amino]-, monohydrochloride (9CI) CN(CA INDEX NAME)

$$\begin{array}{c|c} NH & (CH_2)_5 - CO_2H \\ H_2N - C & C1 \\ O & H_2 - O \\ Me & O \end{array}$$

● HCl

189339-46-6 CAPLUS RN

Hexanoic acid, 6-[[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-CN(trifluoromethyl)phenyl][(2-chlorophenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

189339-47-7 CAPLUS RN

1-Piperidinecarboximidamide, 4-[[3-[[(2-chlorophenyl)sulfonyl](1-CNmethylethyl)amino]-5-(trifluoromethyl)phenoxy]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN189339-48-8 CAPLUS

Glycine, N-[3-[[1-(aminoiminomethyl)-4-piperidinyl]methoxy]-5-CN (trifluoromethyl)phenyl]-N-(phenylsulfonyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$F_3C$$
 $O-CH_2$ 
 $O-C$ 

● HCl

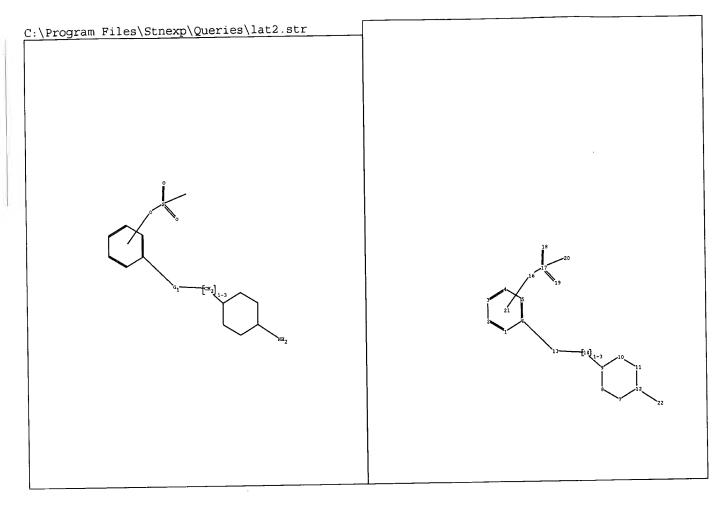
RN 189339-49-9 CAPLUS
CN 1-Piperidinecarboximidamide, 4-[[3-[[(2-chlorophenyl)sulfonyl]amino]-5-(trifluoromethyl)phenoxy]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NH} \\ \parallel \\ \text{H}_2\text{N-C} \\ \text{N} \\ \text{CH}_2\text{-O} \\ \text{O} \\ \text{CF}_3 \\ \end{array}$$

● HCl

RN 189339-50-2 CAPLUS
CN Glycine, N-[[1-(aminoiminomethyl)-4-piperidinyl]methyl]-N-[3-[[(2-chlorophenyl)sulfonyl](phenylmethyl)amino]phenyl]- (9CI) (CA INDEX NAME)

RN 189339-51-3 CAPLUS
CN Benzenesulfonic acid, 2-chloro-, 3-[[1-[imino[(methoxycarbonyl)amino]methy 1]-4-piperidinyl]methoxy]-5-methylphenyl ester (9CI) (CA INDEX NAME)



```
chain nodes :
  13 14 16 17 18 19 22
ring nodes :
  1 2 3 4 5 6 7 8 9 10 11 12
ring/chain nodes :
   20
chain bonds :
   6-13 9-14 12-22 13-14 16-17 17-18 17-19 17-20
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
   6-13 7-8 7-12 8-9 9-10 10-11 11-12 12-22 13-14 16-17 17-18 17-19 17-20
exact bonds :
   9-14
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
```

### G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS

$$\begin{array}{c|c} O & NH \\ \parallel & \parallel \\ MeO-C-NH-C \\ \hline \\ O & CH_2-O \\ \hline \\ Me \\ \end{array}$$

189341-58-0P ΙT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [(N-amidinoazinyl)alkoxy]phenyl benzenesulfonates and analogs as protease inhibitors)

189341-58-0 CAPLUS RN

Glycine, N-[[1-(aminoiminomethyl)-4-piperidinyl]methyl]-N-[3-[[(2-CNchlorophenyl)sulfonyl](phenylmethyl)amino]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{HN} & \text{O} & \text{CH}_2 - \text{Ph} \\ & \text{H}_2\text{N} - \text{C} & \text{CH}_2 - \text{O} - \text{C} - \text{CH}_2 \\ & \text{O} & \text{CH}_2 - \text{N} & \text{O} \end{array}$$